

# Virtual NMR at the HFMRF

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*provides state-of-the-art nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) instrumentation for determining molecular structures that impact environmental remediation and biological health effects.*

## ► Instrumentation

- Twelve NMR spectrometers (ranging from 900 to 300 MHz) and one pulsed EPR spectrometer, with capabilities in high-field liquid-state, solid-state and micro-imaging techniques
- Combined optical and magnetic resonance microscope
- Low temperature probes for metallo-protein chemistry and structure
- High temperature probe for catalytic materials
- Virtual NMR capability to enable use and collaboration with EMSL scientists by remote users

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## Science Areas

### Solution-state

- Structural Genomics
- Biomolecular complexes
  - Nucleic Acids/Protein
  - Protein-Protein complexes
  - Protein-Lipid complexes

### EPR

- Metalloproteins
- Membrane proteins and
- redox chemistry mechanisms
- Catalytic RNA's

### Solid-state

- Metalloproteins
- Solid-state materials research
  - - catalytic, ceramics, amorphous materials.
  - - emerging in biological solid-state research.
- Environmental chemistry
- Actinide chemistry

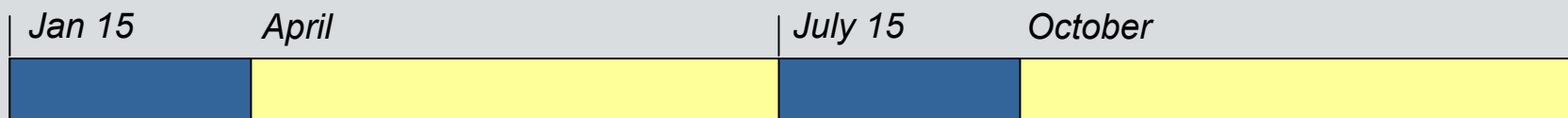
### MR Imaging/ Microscopy

- Imaging and metabolic “signatures” of cells/tissues and organisms.
- Flow and transport-
- Polymer aging
- Methods development
  - - Slow-MAS
  - confocal microscopy

## Proposal Process

*The primary objective is to facilitate the best possible science.*

- ▶ Open call twice a year (1800 recipients)
- ▶ Submitted online via the EMSL User System
- ▶ Proposals reviewed
  - EMSL staff
  - External panel
- ▶ Review criteria:
  - Scientific Merit
  - Appropriateness of the requested instrumentation
  - Relevance to the EMSL/DOE Mission
  - Contribution staff can have in bringing that science to fruition





# Virtual NMR Access at HFMRF

- ▶ Secure, remote operation of spectrometers via internet
- ▶ Live consultations using collaboration tools
- ▶ Reduced travel costs and more flexible scheduling
- ▶ ~20% of facility users elect to use remote access tools



## Publications:

Hoyt, D.W., et al. (2004) "Expanding your Laboratory by Accessing Collaboratory Resources". *Analytical and Bioanalytical Chemistry* **378** (1): 1408-1410.

Chin, G., et al. (2002) "Social Networks in the Virtual Science Laboratory". *Communication of the Association for Computing Machinery* **45** (8): 87-92.

Keating KA, et al. (2000) "Development and Use of a Virtual NMR Facility", *J. Mag. Res.*, **143** p. 172-183.

# Virtual NMR Access at HFMRf

**U. Washington** - G. Varani  
Structure of telomerase  
RNA and telomeric proteins

**Montana State U.** - Valerie Copie  
Three Dimensional Solution  
Structure of NoSL

**Wayne State U.** - J. Wang  
Structure of  
Apo-Lp III/HDL Particles

**Cornell** - Chih-hsin Cheng  
Properties of Surface  
Functional Groups of Black  
Carbon

**Princeton** - F. Hughson  
Intracellular Protein  
Transport

**CWRU** - F. Sonnichsen  
**Vanderbilt** - Sanders  
100 KDal Membrane-  
Bound Enzyme Complex

**U. Central Florida** - L. An  
Amorphous SiAlCN  
Ceramics

**U. Kansas** - C. Larive  
**Wichita State** - W. Carper  
Fulvic Acid-Heavy Metal Complexes

- ▶ HFMRF: 12-NMR spectrometers, 1-pulsed EPR

- ▶ 900 MHz NMR

  - High Resolution liquids – structure of complexes

  - Solid State – optimal for quadrupolar nuclei and biological solids

  - 63 mm bore – optimal for solid-state/ imaging projects

- ▶ Cold probes

  - 2 - 600 MHz now available to users

  - 800 MHz delivery (9/15/05)

- ▶ Next call for proposals (due 01/15/06)

- ▶ Remote access to operate instruments with staff